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The Validation of Pesticide Leaching Models

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Abstract: The validation of pesticide leaching models presents particular problems where the number of model predictions is far in excess of the observed data. Normally, however, there are more frequent field observations for other parameters (notably the site hydrology) than for pesticide concentrations in either water or soil. A five-stage validation procedure which takes advantage of the most frequently available observations and which tests each of the components of the model in a cumulative way, is thus advocated:
Stage 1: Parameterisation of the model using only independently measured parameters.
Stage 2: Hydrological validation: the validation of the predictions of water movement and water content of the soil.
Stage 3: Solute movement validation: where field data are available for solutes other than pesticide, the model should first be validated for them, especially if they are more abundant than the pesticide observations. Conserved solutes such as chloride or bromide are preferred, although nitrate may be used for short periods.
Stage 4: Pesticide fate in the soil: models should use parameters of pesticide fate derived from independent studies.
Stage 5: Pesticide leaching: only in the last stage are the relatively small number of pesticide observations compared with the model predictions with respect to patterns and orders of magnitude of occurrence.
With this scheme, the results of each stage are carried forward to the next, and confidence in the model is built with each stage. This is illustrated using the CRACK-P model and hydrological, nitrate and pesticide data from the Brimstone Farm Experiment Oxfordshire, UK.

Key words: model validation, CRACK-P model, hydrology, macropores

1 BACKGROUND

Leaching of pesticides from agricultural land to surface and ground water is the subject of much current research. Frequently, these studies seek to build models that predict the losses of a pesticide to the surrounding environment. Such predictions are required for a variety of purposes:

To inform crop management practices
For regulatory use
To aid understanding.

Users wish to know how good such models are, and the degree to which they can trust the results. The procedure for building confidence in those results, the process of model *validation*, is however far from certain. This paper suggests ways of improving the validation technique and outlines some of the problems encountered.

Validation is the essential procedure of making sure that the model reproduces the behaviour of the system it tries to mimic. We adopt the terminology established by Fishman & Kiviat,[1] Van Horn[2] and Mihram[3] that

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model *verification* is concerned with the correct function of the algorithms and coding within the program, and that *validation* asks how far the model reproduces the system of interest. Validation is thus a matter of acquiring confidence that the model is an adequate surrogate for the real situation. It concentrates on the issue of testing model performance in the context of the 'training' data set.

A major problem in many pesticide leaching studies is the scarcity of observations available for testing the model. Our proposed procedure is based on the fact that leaching is essentially a hydrological process, and can use much more frequent hydrological data to test individual components of the model independently. We therefore advocate a multi-stage cumulative validation procedure, beginning with hydrological validation.

1.1 Validation in modelling studies

Modelling is in essence a problem-solving activity. Models are built to mimic the behaviour of a particular system, in the hope that they can be used to predict the behaviour of the same system in new situations. Models are frequently developed and tested within the context of an initially data-rich situation (the 'training data set'), before being applied to other situations which have not been observed. In order to answer questions about the behaviour of the 'target' situation with an acceptable degree of accuracy, models may not need to reproduce the behaviour of the 'training' data set exactly. Thus for pesticide leaching models we may be content with a model that will predict the likely magnitude of leaching risk for a new compound, or the semi-quantitative impact of an alternative management regime.

The problem-solving nature of the modelling exercise imposes another constraint: models must be sensitive to parameters which describe the processes that we wish to investigate. Models are essentially simplified abstractions that we choose to study because they are easier to manipulate than the real system. The process of abstracting the model from the complexity of reality therefore concentrates on the topics that are useful in achieving the aims of the modelling study. Thus we are likely to be concerned with time and rate of application of a pesticide, but not with the colour of the tractor used!

1.2 The context

This paper discusses validation within the context of a study of the leaching of pesticides from cracking clay soils. This required the development of a new model, CRACK-P,[4] with the three-fold aims of:

- Understanding the processes involved,
- Prediction of the fate of new and as yet untested compounds,
- Predicting the impact of management practices on the leaching risk.

The study used results from the Brimstone Farm Experiment, in particular the pesticide leaching results described by Harris *et al.*[5] We concentrated on predicting the fate of the herbicide, isoproturon, which was applied on 8 October 1990, and its subsequent fate and appearance in drainage water in the following winter.

The Brimstone Farm Experiment has been used for many investigations into the movement of water and solutes in cracking soils.[6,7] The soil of the site is a pelostagnogley of the Denchworth series,[8] which typically has 55–60% clay and extensive macropores. Effective drainage is required for the utilisation of this soil for arable agriculture; this is achieved by the use of mole drainage, which both introduces close-spaced drainage channels and increases the macroporosity. The Brimstone Farm site has been intensively monitored since its establishment in 1978, and offers a unique facility of 20 field-scale plot lysimeters. The combination of detailed soil physical information, a complete description of the site hydrology and detailed cropping information makes this an ideal context for modelling studies. However, even in this data-rich environment, there were considerable problems with validation.

The data from this site include the continuous measurement of all water leaving the plots in drainage or surface water systems. These systems are sampled for nitrate concentrations and in recent years also for pesticide concentrations. Although nitrate analyses are cheap and can be carried out every three hours, pesticide analyses are necessarily much less frequent, because they are slow and expensive. Detailed data on soil water table position, soil moisture content and all cropping operations are also taken on a routine basis.

The model identified for use at this site was CRACK[9] which was developed explicitly for macroporous soils. CRACK conceptualises the soil as layers of aggregates. Within each layer, the soil porosity is divided into two components, macro- and micro-pores. Water flow into the macropores is generated at the surface by an infiltration excess and, once in the macropores, water moves rapidly downwards. The model allows for drainage of water from the macropores, and so gives an opportunity to model the mole-drainage system that is installed at Brimstone Farm. In CRACK, the macropores are defined by the inter-ped boundaries and, the movement of water and solute into the micropores is described by infiltration theory; water moves into the peds by sorption only and is extracted by the crop. The important term describing the rate of interaction between the macropores and the peds is derived from observations of ped size, or its inverse, crack spacing. Measurement of ped sorptivity unmodified by macropore flow, required by this model, has been described by Leeds-Harrison *et al.*[10] who used a stainless steel tube to infiltrate water into initially air-dry aggregates over a

small circular area having a radius between 1·45 and 2·5 mm.

The CRACK model (as described by Jarvis[11]) includes a description of the movement of a conserved solute, which has already been shown to offer a good description of both the hydrology and the short-term behavior of nitrate at the Brimstone Farm site.[12] A pesticide module was added to the CRACK model, based on the descriptions contained in the CALF model of Nicholls *et al.*[13] as modified by Walker.[14] The combined model is now called CRACK-P. Degradation is modelled as an exponential function, with coefficients dependent on temperature and moisture content. Soil temperatures are estimated from air temperatures using the techniques of Walker & Barnes.[15] The impetus for the work in this paper was the need to test the results of this new model.

2 THE PROBLEM

Model validation studies require large amounts of data, both input data to describe the system being modelled, and output data for validation studies. Basically the process of model validation involves placing the model results beside the observations, and then judging whether the model represents these observations adequately. Although this paper concentrates on the issue of output data, we first record the problems with input data that had to be resolved.

2.1 Input data

Soil properties are notoriously difficult to characterise. Even those properties that remain constant over longer periods of time are subject to sampling variability, which reflects both the inherent variability of the material itself and measurement error. For the Brimstone Farm site all the relevant parameters have been recorded, but for other sites techniques for estimating missing parameters may need to be adopted.

Equally, the meteorological inputs needed to drive the models are not entirely problem-free. For example, there were as many as nine rain gauges operational on the site at any one time. These showed up to 10% variability in rainfall across the site. The problem facing the modeller was the choice of which data set to use. In practice a 'standard' set of agreed rainfall values was used, but the variability indicates some uncertainty with even the most basic input data. Lack of fit between the model results and observations could therefore partly arise from incorrect specification of inputs. The problem is further increased when the model requires derived parameters for which alternative calculation schemes are available; Reference Evapotranspiration, ET_0, is a typical example. For this study we used the MORECS[16,17] method applied to the data from the nearby (15 km) Brize Norton meterological station, to give a crop-sensitive estimate of ET_0.

The defeatist may decide that if there are problems with the input data, then modelling is impossible. However, the choice of the input data can be seen as part of the abstraction process, in which the modeller chooses both the processes and the parameters necessary to build the model.

2.2 Output data

Validation strategies involve comparisons between the observed data and the predictions of the model. This is a basic problem for validation of pesticide leaching models, because pesticide data are inevitably sparse and much less frequent than either observations of other variables, or predictions from the model. Table 1 illustrates this problem by listing the number of observations and model predictions for the Brimstone Farm site for a 120-day period. In this example drain flows are recorded every half-hour, water tables every hour and nitrate concentrations every three hours. However, because of the large analytical effort to determine the pesticide concentrations in both soil and water samples (documented for example by Harris *et al.*,[5] pesticide concentrations are available for no more than 20 to 30 samples per plot, and as a result the number of data points available for model validation is small. By con-

TABLE 1
Numbers of Observational Data Points and Model Prediction Points for an Example 120-Day Period for One Plot at the Brimstone Farm Site

	Number of days with observations	*Data points per day*	*Number of data points*	*Number of model predictions*
Water discharge	120	48	5760	5760
Water table	120	24	2880	5760
Nitrate concentration	120	8	960	5760
Pesticide in drainflow			20–30	5760
Pesticide in soil	6	6	36	17280

trast, the model is capable of predicting the pesticide concentrations in the drainage water and in every soil layer at every model increment (normally every half-hour).

The problem is thus to devise a procedure to establish the goodness of fit of the model in which the number of model data points roughly matches the number of observations for some components of the model (e.g. the hydrology) but is markedly different for others. This problem is made worse by the fact that the pesticide data are also the most important as well as the most sparse. Model validation must take note of the relative importance of these sparse data points.

3 VALIDATION STRATEGIES

Three solutions to the problem of model validation are perhaps possible. We term these: blind mechanism, global validation and multistage validation. These are examined in turn.

3.1 Blind mechanism

This approach assumes that if we understand the physics, and if we can measure the parameters correctly, then the results of the physically based models must be right. This method is useful in deriving the idealised behaviour of materials under reference conditions, but it does not attempt validation as such. Rather it states that where the behaviour of the observed system deviates from the modelled behaviour, these anomalies can indicate and identify complications in the real system. This method works well for simple systems. For example, in astronomical studies, the deviation of one planet from its orbit has been used to demonstrate the existence of another. Where the system is simple, then deviations between model and reality are likely to have significance.

In the context of pesticide leaching studies, an example of the mechanistic approach might be the use of the combined Richards' equation and the convection-dispersion equation.[18] Such models are useful in determining theoretical transport in soils, but they are difficult to transpose to real field situations where the assumptions, particularly that of a uniform homogeneous medium, are seldom realised.

3.2 Global validation

The standard statistical approach is to develop some global function of the differences between observed and predicted behaviour. Such procedures seek to describe model performance using a 'Goodness-of-Fit' statistic (GOF) of the form:

$$\text{GOF} = \sum_{\text{Variables}} \sum_{\text{Time}} \text{f(Observed, predicted)}$$

where the sum is taken over all the observational points (times) and over all the variables for which there are both observations and predictions.

It is possible to establish a variety of functions to represent the effects of the differences. A number of such statistics applicable to pesticide leaching studies are described by Walker *et al.*[19] A popular function from classical statistics is the sum of the squared differences (the error):

$$\text{Error} = \frac{1}{\text{NT}} \sum_{\text{Variables}}^{\text{N}} \sum_{\text{Time}}^{\text{T}} (\text{Observed} - \text{Predicted})^2$$

However, this statistic has problems. It gives equal weight to all points, and it does not take into account any error in the observations, although this particular problem may perhaps be circumvented by using the techniques described by Whitmore,[20] who partitioned the modelling error into those differences between the lack of fit between prediction and the mean of replicate measurements, and the 'pure' error associated with the variability within each set of measurements. This technique is, however, only applicable where strictly replicated measurements are available. Hydrologists have identified a number of alternative GOF statistics (see the reviews by James and Burges[21] and Loague and Green).[22] Thus for example it is possible to weight the calculation in some way so as to concentrate on key variables, or key points in the observations (such as peaks).

In many models, the statistic is simplified by restricting the number of variables used to define the error sum, and in particular to concentrate on critical output values. This procedure has the danger that an incorrectly specified model may fortuitously give correct output values but entirely misrepresent the internal workings of the system. Such models may then reproduce the behaviour of the training data set, but give erroneous predictions for other data because they fail to represent the mechanisms operating.

The use of a goodness-of-fit statistic is popular where the aim is to 'fit' the model by altering the parameters in such a way as to minimise the error function. If the model is linear, and the errors are independent and normally distributed, then minimising the error becomes a simple regression exercise. However, many models are non-linear and their errors non-normally distributed, so alternative optimisation algorithms are required (e.g. Klepper & Hendrix).[23] Such 'fitted' models have parameters that are not independent of the training data set from which they were developed, and are thus difficult to apply outside that training data set.

The major problem encountered when attempting to use an error statistic for the optimisation of pesticide leaching models is the extreme mismatch between the number of observations for each variable. Thus, if the model were optimised against the data described in

Table 1, two situations could arise:

(a) Using both the hydrological observations and the pesticide data would fit the model to 5640 hydrological data points, but only 30 pesticide observations. The resultant goodness-of-fit statistic would reflect the hydrological component of the model almost exclusively, and the difference between good and poor fits to the pesticide fate model would be virtually undetectable.

(b) If the goodness-of-fit statistic were weighted to reflect the relative frequency of the observation points, the weights would be in the ratio 1:2:2000 for the discharge, water table and pesticide concentrations respectively. The use of weights with such discrepant values is, to say the least, uncomfortable, and is likely to lead to uncertain results.

Lastly, such an error analysis takes no account of the fact that the observations are not independent, but form a sequence in time and, frequently interest focuses on the nature, and in particular the pattern of that sequence. This is a recurrent problem in hydrological studies, in which a model that predicts the peak flow volume of a runoff event well in terms of volume, but slightly offset in time, will appear, in goodness-of-fit terms, to be less good than a model which predicts the flow at the correct times but incorrectly predicts the volumes. The choice between a concern for timing and values is often critical in hydrological studies, and the same is generally true of pesticide leaching models. For prediction of pesticide leaching risk, it is usually the peak concentrations that are of critical concern, and over a period such as a whole winter then a timing difference of a few hours is of little consequence for the interpretation of the results, though it may have a major effect on the goodness-of-fit statistic.

3.3 Multistage validation

The last procedure, which we shall describe in detail, we term 'multistage validation' (although the term 'multicomponent validation' would have been equally appropriate). In this, the model is validated one component at a time, and the validation confidence is carried forward. This validation strategy is thus a sequential process, which evaluates each component of the model separately and sequentially, not a single once-and-for-all process at the end of the modelling exercise. The number of different data points available for each stage is then addressed separately, rather than trying to wrap the whole exercise into a single overall 'goodness-of-fit' statistic. Although we present the strategy as a strict sequence, the order is, to a degree, variable, and depends on the availability of the relevant data for each component. Nevertheless, we suggest that this is probably an accurate reflection of actual modelling practice.

Stage 1: Parameterisation of the model using independent measurements

From the outset, any model validation exercise should be based on independent physical parameters. This places significant requirements on the data set used to verify the model. It also places constraints on the model itself, in that it requires that the parameters are capable of measurement. If a model contains parameters that are unmeasurable, and so can only be fitted retrospectively, in a strict sense the model can never be independently validated.

The first stage of the model validation procedure must then be a review of the data available, and the selection of a definitive set of parameters. It is possible at sites of the complexity of Brimstone Farm, where detailed soil investigations have been undertaken over 17 years, to find alternative measurements for essentially similar parameters, perhaps taken at different times, or by using different techniques. Where these data are used for model validation, the choice of a parameter set to represent the site must be taken *a priori*, and not retrospectively 'tuned' to make the model fit better.

This choice of input data is particularly difficult and to some degree it is a matter of skill and intellectual honesty on behalf of the modeller which it is not possible to formalise. Walker *et al.*[19] noted that different modellers, given the same scenarios and working with the same models, produced different results, which was in part a result of their different subjective choices of key input parameters. However, some guidance can be established by requiring that all input data are within the known range for the values. Consequently, the use of a parameter data base to develop expected characteristics is recommended. Where multiple measurements are available, the use of mean values will do much to ensure consistency.

Equally difficult is the situation where parameters are not available. It is particularly easy to have parameters in models that cannot be measured directly or for which very few measurements have been made. In these cases, use of model default parameters is recommended, and other values should be used only if there are good, physically based, arguments for them.

However, once chosen, the input parameters must be both explicitly defined and remain unchanged. If at later stages in the modelling process, it is suggested that some input parameters are incorrectly specified, then the review of their values need to be undertaken outside the modelling procedure, and the validation process restarted from the beginning.

Stage 2: Hydrological validation

Leaching is essentially a hydrological process, and any validation of a leaching model must first reproduce the

hydrology of the site. A common error in the use of leaching models is to optimise a complex model against a small number of observations, so ending up with a set of parameters which fortuitously match observed pesticide data, but which in fact fail to represent the hydrology.

There are generally two components of site hydrology: the soil water status and the fluxes of water through the profile (although these are of course related). In general, the model needs to be validated against both of these conditions. A successful pesticide leaching model would be expected to predict both of them. If the fluxes predicted by the model are not correct, then estimates of pesticide movement will themselves be incorrect: the concentrations may be right but the total fluxes will be wrong, or vice versa. Only if the water fluxes are correct is it possible to calculate both the concentrations and the fluxes of the solute correctly.

This stage in model validation is normally relatively easy to undertake technically, where there are independent measurements of soil hydrological status. The validation of site hydrology may use some of the statistical goodness-of-fit techniques, and there is generally no major problem where the number of observations is of the same order as the predicted points.

Testing the soil moisture component is less easy, except in soils with a fluctuating water table. In these soils (such as the one at Brimstone Farm) the hydrological status of the soil can be summarised by the position of the water table, and this can be recorded frequently using piezometers, autographic water table meters or capacitance probes. In more permeable soils, soil water measurements, such as those obtained using a neutron probe, are less frequent, and again a procedure for validating a large number of model predictions against a small number of observations is required.

This hydrological verification is illustrated by Fig. 1, which shows the observed drain discharges and water table positions for the Brimstone Farm site, plus the predictions from the CRACK model. It was because CRACK gave such good predictions of the site hydrology that it was developed as a pesticide leaching model for the site.

However, even here difficulties were encountered. It has been repeatedly observed that the timing of the first major storm event sufficient to produce drainflow has a significant impact on the quantity of solute (including pesticide) leached (see, e.g., Rose *et al.*).[24] It was therefore important that the model predicted the return to field capacity accurately, and so considerable effort was necessary to identify both the initial soil moisture conditions and the values of actual evapotranspiration during the autumn period.

Stage 3: Solute movement validation

If at all possible, the solute movement component of the

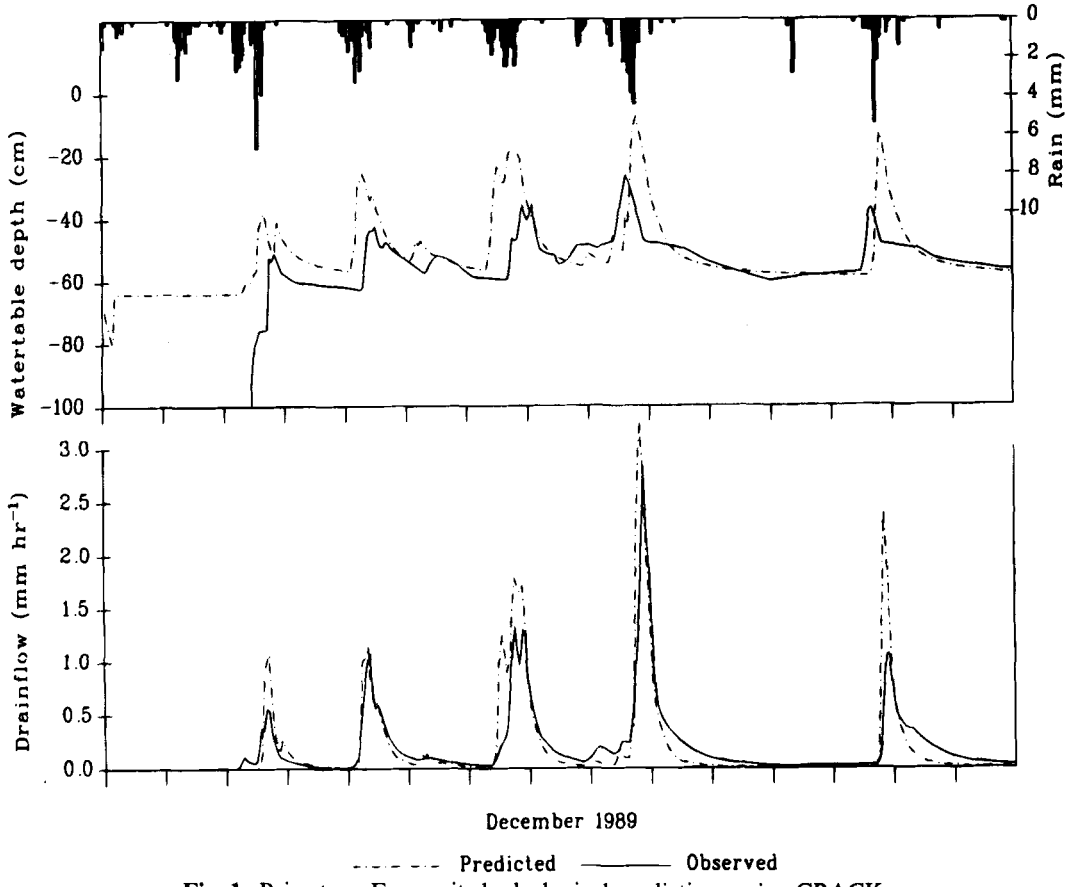

Fig. 1. Brimstone Farm: site hydrological predictions using CRACK.

model should be independently tested in a similar way. Measurements of some ions can be made easily, quickly and cheaply, and so it is often possible to collect a sufficient density of data points to test the model rigorously. Where data permit, the model should thus be tested for solutes other than pesticides. The use of a conserved solute such as chloride or bromide is recommended. Because it is slowly generated in the soil by mineralisation of organic matter, and is also slowly taken up by plants or lost by denitrification, nitrate is less suitable. However, when temperatures are low and mineralisation, crop uptake and denitrification rates are also low, then nitrate can be treated as a conserved solute for short periods.

For the Brimstone Farm site it was possible to use the observations of nitrate concentrations in the drain water over a 10-day period in December 1989 to establish a test of the CRACK model (Fig. 2). The model predicts the pattern of dilution over rainfall peaks very well. The initial mismatch between observed and predicted is due to the problem of identifying the correct initial conditions, and does not invalidate it for the current purposes. Where the model predicts the correct pattern of solute movement, it can be argued that the model correctly reproduces the processes within the soil.

Stage 4: Fate of pesticide in the soil

All pesticide leaching models require some component to describe sorption of the pesticide onto the soil and its subsequent degradation by microbial activity, such as estimates of K_d and half-life. However, estimation of these parameters is often far from straightforward. In particular the half-life needs to be estimated from incubation studies that relate to the properties of the site in question. For validation, it is important that models should use parameters obtained from independent derived studies. It is fortunate that for the Brimstone Farm site, the studies of Nicholls *et al.*[25] provide this independent measurement of the crucial parameters.

Stage 5: Pesticide leaching validation

Only in the last stage can the relatively small number of pesticide observations be placed against the predictions. Once it has been established that the model predicts the site hydrology and solute concentrations, then it is possible to evaluate the predicted pesticide losses. Because the observations are costly, the number of data points is usually small. Model predictions are generally acceptable if they are within an order of magnitude of the observations, and in particular if they match the observed patterns of behaviour.

An example of this last stage is seen in Fig. 3. This shows that both the values and the patterns of pesticide concentrations in the drainwater at Brimstone Farm are predicted moderately well by the CRACK-P model.

Although this validation strategy suggests a strict sequence, the practical reality is more fluid. Some stages, particularly the validation against solute data,

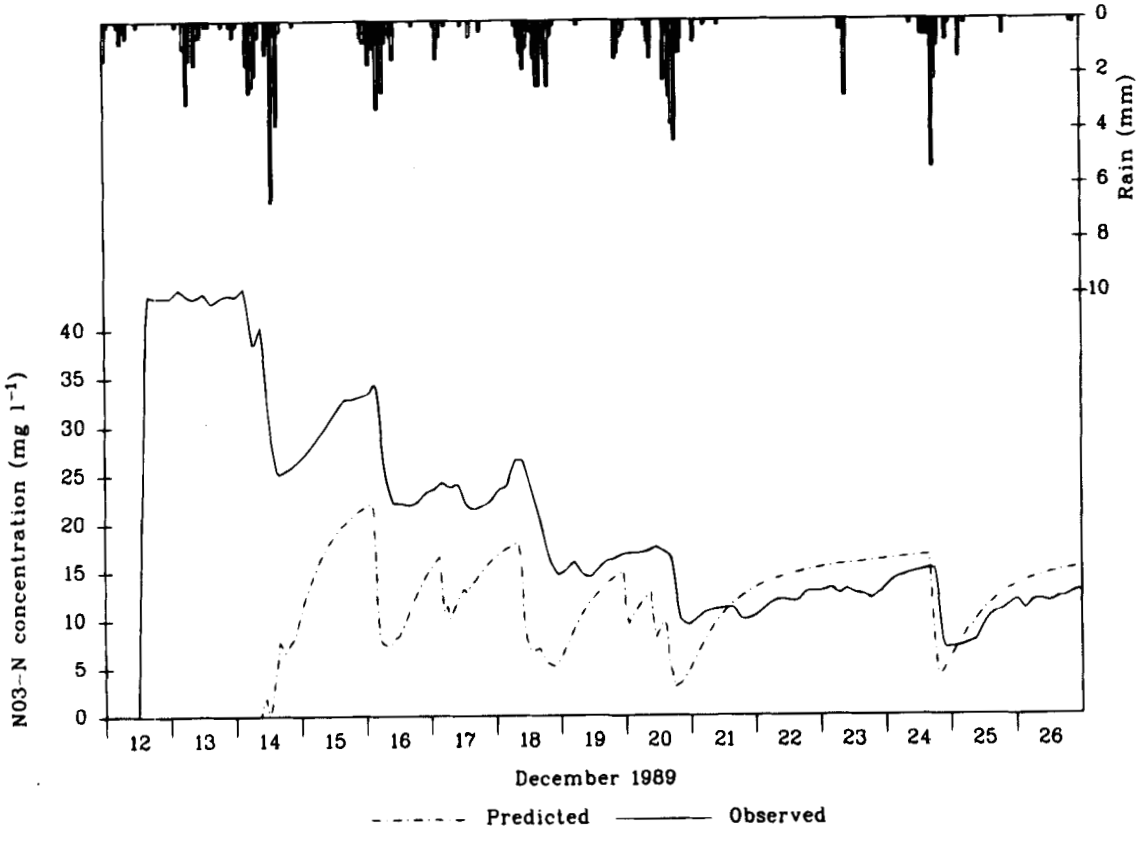

Fig. 2. Brimstone Farm: predictions of nitrate leaching, December 1989.

may not be possible if the data are not available. Equally, the collection of independent parameters for both the soil physical properties and pesticide fate in soil need not adopt the exact sequence of steps but may be continued right through the modelling process. At the same time, each of the procedures can raise issues which go right back to the pre-validation stage, which is the specification, abstraction and derivation of the model. Thus, for example, examination of the soil physical conditions will indicate the sort of model that is likely to be appropriate (including, for example, the question as to whether the soil has a significant preferential flow component requiring a macropore model); and the success or otherwise of the hydrological and solute leaching components will indicate the overall match between the model choice and the physical condition it represents. At each stage the modeller will have the opportunity to re-examine the nature of the model that is being used, and, if appropriate and possible, to make appropriate choices in model implementation, or even to alter the model itself. In this way, the continuous feedback between model and reality[26] is maintained. Only if the model is prescribed *a priori* and cannot itself be modified, as in some registration studies, will a strict adherence to the strategy be required. Nevertheless, however the sequence of stages is approached, the principle should be maintained that the individual components of the model, and in particular the hydrological component, should be independently validated in advance of the validation of the pesticide leaching results.

4 CONCLUSIONS: THE USE OF MODELS

A successful pesticide leaching model that has passed through all these validation stages should predict both the site hydrology (the water balance and the water discharge) and the pesticide losses using parameters that have been derived independently of the model, and with no retrospective 'fitting of parameters'.

Although the validation of pesticide leaching models is difficult, the validation procedure differs from later 'application' uses of the model, where estimation procedures to derive parameters is permissible. Once accepted, a model does not necessarily need to be repeatedly re-validated. 'Application' uses of the model may, for example, adopt less stringent procedures for estimation of parameters, such as the use of pedotransfer functions to estimate the water retention and hydraulic conductivity functions.

Nevertheless, there is another sense in which every

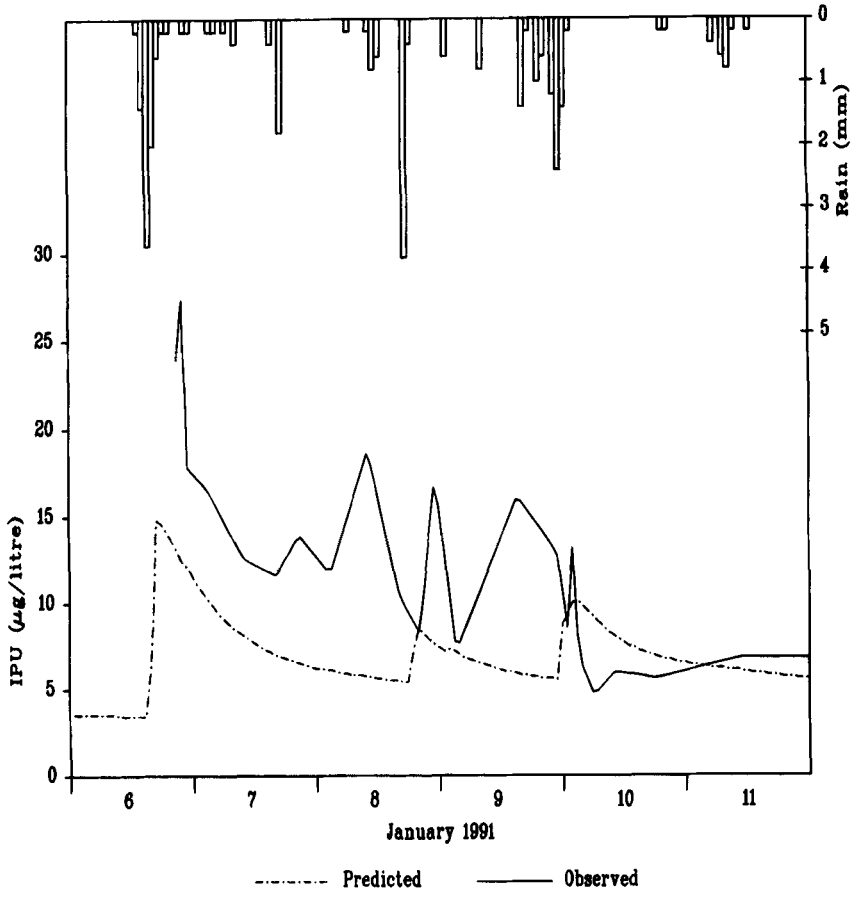

Fig. 3. Comparison of observed and predicted isoproturon (IPU) concentrations in drainflow at Brimstone Farm, January 1991.

use of the model has some element of validation. Where the model produces results that are unexpected, or do not fit the site details, then its status may be questioned. Frequently the problem is inadequate identification of the correct model for the site, but the possibility of error in the model should never be overlooked. As the modelling community uses a model repeatedly, and it becomes accepted, the cumulative experience gives it a different validation, which is derived from repeated testing. Few pesticide leaching models (indeed few soil or hydrological models) have that sort of status at present.

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